Los Alamos National Laboratory
Theoretical Division Special Feature

T-1
Equation of State &
Mechanics of Materials

Modeling Metallic Microstructure Using Moving Finite Elements

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To attack the general problem of evolution of metallic grain microstructure in 3D, we employ two different methods: using Monte Carlo (MC) techniques to anneal an effective discrete model on a fixed lattice [1], and using Gradient Weighted Moving Finite Elements (GWMFE) to evolve grain boundaries by mean curvature (local velocity proportional to the local curvature) – the simplest continuum model for grain evolution [2,3]. These two models reduce to each other in the appropriate limits. MC has the advantage of computational and algorithmic simplicity while GWMFE is more easily adaptable to including coupled transport fields such as vacancies and impurities, and other geometrical and physical complexities occurring in the simulation of interconnect-via interactions as related to electromigration reliability of submicron integrated circuits. Cross comparisons of the two calculational techniques will produce the best synthesis of accurate physical models and computational speed. We also compare to other methods, such as 2D front-tracking [3].

As an example of MC grain evolution in the confined geometry of an Al interconnect on a semiconductor chip, we have evolved an initial microstructure of randomly oriented grains on a fixed lattice using a discrete effective classical spin model originally developed to model magnetic domains (Potts model) [1]. For the first few time steps, MC scales with the number of volume points. Activity binning and N-fold or cluster flip MC techniques allow significant speed-ups in the time evolution [1]. (Incorporation of volume information may reduce the amount of these speed-ups.) We evolved both a regular fcc lattice, where discreteness trapping is not a problem [1], and unstructured grids resulting from the LANL X3D code, where we see from Fig. 1 that 5th neighbor interactions are needed in order to get normal grain growth without pinning at finite grain size. We are investigating how various algorithms for treating further neighbors effect these MC grain growth statistics. Having the ability to use the MC code on the X3D generated geometries and meshes will greatly enhance it's usefulness as a tool to generate initial conditions for the GWMFE code.

Fig. 1. Mean grain size normalized to the total volume as function of time and number of neighbors N from Monte Carlo evolution of the Potts model [1] on an unstructured grid generated by the LANL X3D grid code. Note growth stagnates for N<5.

In the finite element approach, we represent the metallic grains on an unstructured tetrahedral mesh, generated using the LANL X3D grid code. We use an implicit implementation of the GWMFE method to move the grain surface (interface) triangles. Although volumes are deformed by the moving grid, the computational complexity of the method is only 2D, not 3D, because GWMFE moves triangles, not tetrahedra [2]. Fig. 2a shows an intermediate microstructure, with the average grain size approximately half the width, resulting from MC evolution on an underlying fcc grid, which we used as input to GWMFE. After a few GWMFE time steps, the initially jagged interfaces between the grains (a consequence of the fixed lattice used in the MC simulation) have begun to smooth out under the action of mean curvature motion (Fig. 2b). In Fig. 2c, GWMFE has evolved the microstructure to a completely smooth state. Visible in the interior, due to one of the foreground grains being made "semitransparent", are "triple lines", where three grains meet at 120° angles, and "tetrahedral points" where four

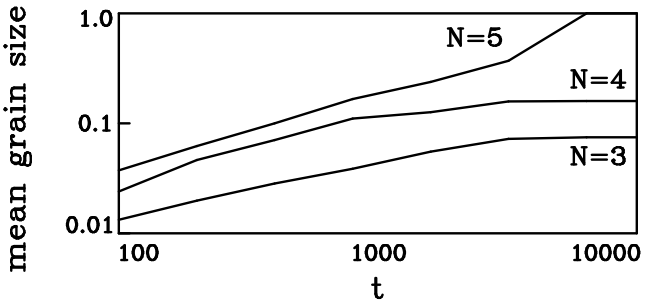
materials meet. On the surface of the geometry, we see that the boundary constraint leads to several triple points (analogous to 2D simulations) where three materials meet at 120° angles. All interface angles agree with predictions for mean-curvature motion. However, the underlying grid (Fig. 2d) composed of interface triangles is becoming distorted, and must be refined in some areas and derefined in other areas. Although the X3D code can accomplish the necessary topological changes in a semi-automated manner at this time, we are currently completing development of a fully-automated topological analyzer called "Graph Massage" which will seamlessly accomplish the necessary topological changes for the simulation to continue while preserving grain interfaces. High level routines detect major topological "events" (such as the collapse of an entire grain, which is then simulated correctly by restricting mesh connectivity changes to only those that sufficiently preserve material volumes). We next plan to investigate grain boundary evolution under isotropic thermal strain starting from initially randomly oriented grains.

To add the capability of correctly modeling grain boundary evolution in the environment of time-dependent stress and strain due to unsteady and spatially nonuniform temperature and impurity gradients, it will be necessary to couple the GWMFE code to a truly 3D physics code. Currently under development for this purpose is the Arbitrary Lagrangian Finite Element (ALFE) code which is a fully-implicit Galerkin Finite Element method for tracking the evolution of fully-coupled systems of partial differential equations. The code under development will use the latest "matrix-free" iterative methods, and thus will be highly parallelizable. The fully-implicit adaptive time-stepping scheme used will allow for efficient resolution of phenomena at various timescales, while access to the X3D adaptive grid refinement capabilities will allow ALFE to track phenomena at various spatial scales as well. Finally we note that ALFE is an "Arbitrary Lagrangian" code, which means it has the capability of correctly tracking the evolution of phenomena in an arbitrary, spatially and temporally nonuniform, coordinate system. This is crucial for the grain growth simulation, where volume tetrahedral movement is "slaved" to the interface triangle movement computed by GWMFE.

We are also currently evaluating a 3D electromigration simulation code from Motorola which will take as input the microstructure from Fig. 2d and predict electromigration reliability for the interconnect being simulated. These studies will establish whether the additional overhead of a fully 3D model is justified, or if 2D simulations [3] adequately describe the evolved microstructure. We expect that 3D models will be important in intrinsically nonplanar geometries, such as vias.

[1] E.A. Holm, Ph.D. Thesis, University of Michigan, 1992, unpublished.
[2] Andrew Kuprat, in the Proceedings of the Fifth International Conference on Numerical Grid Generation in Computational Fluid Dynamics and Related Fields, Mississippi State University, Mississippi, 1-5 April, 1996.
[3] H.J. Frost and C.V. Thompson, J. Elec. Mater. 17, 447 (1988).

Fig. 2. GWMFE evolved microstructure as a function of dimensionless time (surface tension of order 1 and spatial dimensions of order 1): (a) t=0: MC model evolved microstructure used as input. (b) t=0.1: GWMFE has smoothed the initially jagged interfaces. There is otherwise no significant grain boundary motion. (c) t=30: The smooth boundaries allow use of large timesteps in the implicit adaptive GWMFE scheme. (d) Underlying surface grid of triangles at the same time as in (c). (Volume tetrahedra are obscured.) Topological change is necessary at this point.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